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Analysis of Field-Aided, Charge-Coupled Device Transfer

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We study the numerical solution of a nonlinear, partial-differential equation that describes charge transport in a model of a charge-coupled device (CCD). This model differs from previous models in that field-aiding of the transfer is taken into account. Although a derivation of the transport equation is given, the main emphasis in the paper is on the numerical techniques involved, and no actual numbers are presented. Actual numerical results based on the techniques developed here can be found in several recent design studies. The equation, which is parabolic, has one space dimension and one time dimension. Galerkin's method, with standard chapeau functions, is used to discretize in space. This results in a very stiff system of nonlinear, ordinary, differential equations. To solve these equations, we use a first-order backward Euler scheme coupled with extrapolation. A number of alternative schemes were tried and found to be inadequate.

I. INTRODUCTION

In this paper, we study the numerical solution of a nonlinear, partial-differential equation that describes charge transport in a model of a charge-coupled device (CCD). The emphasis is on the numerical techniques involved, although a derivation of the equation is given. The reader is referred to other papers where the solutions are used in device theory and design.[1,2] We briefly summarize the physical background of the equation first.

A knowledge of the dynamics of charge transfer in a CCD is, of course, central to a complete understanding of its operation. A calculation of the motion of charge in a CCD, starting from the coupled, nonlinear Poisson and charge-conservation equations and taking into account the full geometry of the device, has so far proved impossible. However, Strain and Schryer[3] and, independently, Kim and Lenzlinger[4] developed and studied an approximate, one-dimensional model of charge transfer in a CCD. The original analysis considered motion owing only to diffusion and the mutual repulsion of the charge carriers. Field-aided transfer was ignored. Since these original studies, a number of other authors have studied the effects of field-aiding.[5–8] In Refs. 5, 6, and 8, as in the original papers,[3,4] an infinite sink for the charge at one end of a cell is assumed. The assumption of an infinite sink rules out charge "bunching," which in certain situations is an important effect (for an example of this, see Ref. 1, Fig. 8). In Ref. 7, the assumption of an infinite sink is not made. In this paper, we extend the original work[3,4] to include field-aiding and more realistic boundary conditions. Our model can describe both surface[9] CCDs and buried-channel[10] CCDs (BCCDs). We do not include the effects of surface traps, since the main application[1] was to BCCDs. We feel the numerical scheme described here has advantages over that used in Ref. 7, where essentially the same model as ours was used to study surface CCDs, with the effect of traps included. Calculations using our methods show that BCCDs, which can be fabricated with present technology, should be extraordinarily fast and efficient and have reasonable charge-carrying capabilities. Transfer times of 1.8 ns are predicted for a two-phase device having 10-μm-wide electrodes.[1] Slower but similar results are obtained for surface devices.

Strain and Schryer[3] solved, by the method of finite differences, a transport equation quite similar to the one we study here. However, their method of solution proved inadequate when applied to our equation. It is possible to obtain solutions of the transport equation as follows. We use Galerkin's method[11] with standard chapeau functions in space. We treat the time behavior by polynomial extrapolation to the limit of the results of a first-order, fully implicit (nonlinear), finite difference scheme. Although the equation only roughly models the true physical situation, an accurate knowledge of the solution as it varies over many orders of magnitude is necessary if it is to be of any use. This requirement makes the numerical solution of the equation difficult. Many other schemes were tried, and the above method is the only one we found that could solve the problem.

The equation of charge transport is derived in Section II, although some more complex details are given in Appendix A. The technique

for numerically solving the equation of charge motion is given in Section III, with some details in Appendix B. Questions of existence and accuracy are discussed in Section IV, along with the use of polynomial extrapolation. An outline of the theory of extrapolation is given in Appendix C. The method by which initial solutions are obtained is the subject of Section V. Finally, in Section VI we discuss several other schemes by which we tried to solve the equation of charge motion and which failed.

II. DERIVATION OF THE TRANSPORT EQUATION

We refer the reader to the literature for a discussion of the principles of operation of either surface CCDs[9] or BCCDs.[10] Basically, however, both are devices that move packets of charge from under one electrode to under another electrode by suitably changing the voltage on the electrodes.

As in Ref. 3, we assume that the charge can be described by a charge density $q(x, t)$. Here, x is the distance under the plates (see Fig. 1) and t is the time. Then, as we show in Appendix A, the component of the electric field along the direction of motion of the charge, which is due to the mutual repulsion of the charge, is

$$E_x^q = -Sq_x. \tag{1}$$

The elastance S is assumed to be a constant independent of x and t. In all that follows, we use subscripts to denote differentiation; thus, $q_x = \partial q(x, t)/\partial x$, etc. Equation (1) holds for both surface and buried

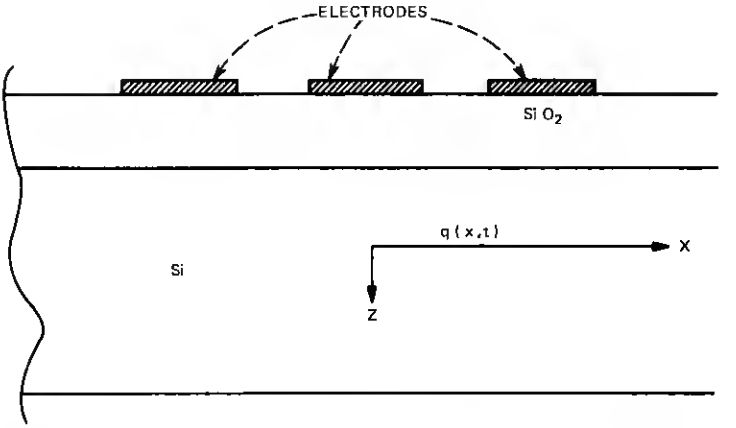


Fig. 1—Schematic of a CCD showing relation to device of x-coordinate in transport equation.

channel devices, although the values of S are different in each case. Expressions for S are given in Appendix A in terms of the physical parameters of the devices.

Let $\varphi(x, t)$ he the given driving potential due to the voltages applied to the electrodes. For a surface CCD, φ is the electric potential at the oxide semiconductor interface, while, for a BCCD, φ is the potential at the potential minimum of the huried channel. In most applications, we have approximated φ hy the potential in the CCD in the ahsence of any mohile charge.[12,13]

The total field along the direction of motion is

$$E_x = -Sq_x - \varphi_x. \tag{2}$$

The current density is[9]

$$J(x, t) = q\mu E_x - Dq_x, \tag{3}$$

where D is the diffusion constant and μ is the mohility, which we also assume to be constant. If we suhstitute (2) into (3) and make use of the Einstein relation $D = (kT/e)\mu = \alpha\mu$, then

$$J(x, t) = -\mu[(\alpha + Sq)q_x + q\varphi_x]. \tag{4}$$

If we substitute (4) into the charge-conservation equation,[14]

$$q_t + J_x = 0, \tag{5}$$

we get the desired transport equation,

$$q_t = \mu[(\alpha + Sq)q_x + q\varphi_x]_x. \tag{6}$$

The appropriate solution of (6) satisfies an arhitrarily given initial distrihution of charge $q(x, 0)$ and the houndary conditions $J(0, t) = J(L, t) = 0$. The boundary conditions state that there is no charge flow into or out of the device at either end. L is the length of the devicc.

It is convenient to write (6) in terms of dimensionless quantities, as in Ref. 3. Let

$$\tau = t/(L^2/\mu v_0), \quad y = x/L, \quad w = Sq/v_0, \quad \Phi = \varphi/v_0, \quad \beta = \alpha/v_0, \tag{7}$$

where v_0 is a reference voltage. Then (6) hecomes

$$w_\tau = [(w + \beta)w_y + w\Phi_y]_y. \tag{8}$$

As it turns out, there seems to be no natural voltage unit in the problem (Ref. 3), so we typically pick $v_0 = 1$ volt.

Physically, the quantity of interest is the total charge present hetween any two points $0 \leqq y_1 < y_2 \leqq 1$. This suggests that, instead of $w(y, \tau)$, we consider

$$Q(y, \tau) = \int_0^y w(\xi, \tau)d\xi. \tag{9}$$

If we integrate eq. (8) with respect to y from 0 to y and make use of the boundary condition $J(0, t) = 0$, we get

$$Q_\tau = (Q_y + \beta)Q_{yy} + Q_y\Phi_y. \tag{10}$$

Since the right-hand side of (10) is just proportional to $J(y, \tau)$, we see that $Q_\tau(1, \tau) = 0$. From this last remark and (9), it follows that the correct boundary conditions on $Q(y, \tau)$ are

$$Q(0, \tau) = 0, \qquad Q(1, \tau) = Q_T = \text{const.} \tag{11}$$

The appropriate initial condition is determined from $w(y, 0)$ by setting $\tau = 0$ in (9). The transport problem we wish to solve is, thus, eq. (10), subject to boundary conditions (11) and given initial conditions. This is a much simpler problem than attempting to solve (8) for the charge density.

III. SOLUTION OF THE TRANSPORT EQUATION

We simplify the notation slightly by setting

$$\psi(y, \tau) = \Phi_y(y, \tau), \tag{12}$$

and note that (10) can be written

$$-\beta Q_{yy} - \frac{1}{2}\frac{\partial}{\partial y}(Q_y)^2 - \psi Q_y + Q_\tau = 0. \tag{13}$$

If we multiply both sides of (13) by a continuous, piece-wise differentiable function $f(y)$ which satisfies $f(0) = f(1) = 0$, integrate the result from 0 to 1, and integrate the terms containing second derivatives by parts, we obtain (letting $f' = df/dy$)

$$\int_0^1 \{[\beta Q_y + \tfrac{1}{2}(Q_y)^2]f'(y) + [-\psi Q_y + Q_\tau]f(y)\}dy = 0. \tag{14}$$

Equation (14) is the starting point for the application of Galerkin's method, because any twice-differentiable function $Q(y, \tau)$ that satisfies (14) for all continuous, piece-wise differentiable $f(y)$ satisfying $f(0) = f(1) = 0$ must also be a solution of (13).

We now discretize in space by introducing a net $\{y_1, y_2, \cdots, y_N\}$ on $[0, 1]$ and a set of standard chapeau functions $f_j(y)$, $1 \leqq j \leqq N$, as pictured in Fig. 2 and defined in Appendix B. In all that follows, the

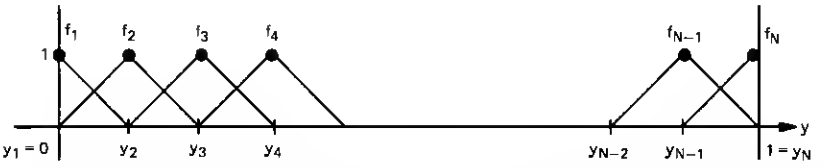


Fig. 2—Discretization of the space interval and the corresponding chapeau functions.

net $\{y_1, \cdots, y_N\}$ is assumed to be given and fixed. In terms of the basic cbapeau functions, we define approximations to the solution and external field:

$$\bar{Q}(y, \tau) = \sum_{j=2}^{N-1} Q_j(\tau) f_j(y) + Q_T f_N(y), \tag{15}$$

$$\bar{\psi}(y, \tau) = \sum_{j=1}^{N} \psi_j(\tau) f_j(y). \tag{16}$$

Note that $\bar{Q}(y, \tau)$ has been constructed to satisfy tbe boundary conditions, $\bar{Q}(0, \tau) = 0$, $\bar{Q}(1, \tau) = Q_T$. The functions $Q_j(\tau)$ are yet to be determined, but we require tbat they satisfy tbe initial conditions

$$Q_j(0) = Q(y_j, 0). \tag{17}$$

Because of (17), $\bar{Q}(y, \tau)$ satisfies the correct initial conditions at tbe mesb points: $\bar{Q}(y_j, 0) = Q(y_j, 0)$. We define $\psi_j(\tau) = \psi(y_j, \tau)$, so tbat $\bar{\psi}(y_j, \tau) = \psi(y_j, \tau)$.

To determine tbe $N - 2$ functions $Q_j(\tau)$, we require tbat $\bar{Q}(y, \tau)$ satisfy (14) for each of tbe $N - 2$ cboices of $f(y)$, $f(y) = f_j(y)$, $2 \leqq j \leqq N - 1$, witb $\psi(y, \tau)$ replaced by $\bar{\psi}(y, \tau)$. This yields a system of $N - 2$ first-order, nonlinear, ordinary differential equations for the $Q_j(\tau)$. This technique bas a robust history and has been applied, not only to many problems of tbe same type as (13), but to otber types of problems as well. The idea is quite simple: Let tbe approximate solution be a linear combination of the functions f_j, $2 \leqq j \leqq N - 1$ and tben make the left-band side of (13) ortbogonal to eacb of tbese functions. In geometrical terms, this means making tbe left-hand side of (13) orthogonal to tbe span of $f_2, \cdots, f_{N-1}$, denoted by $\langle f_2, \cdots, f_{N-1} \rangle$, in $\mathcal{L}^2[0, 1]$ in the usual inner product: $(f, g) = \int_0^1 f(y) g(y) dy$. Then, crudely speaking, as more points y_j are cbosen, $\langle f_2, \cdots, f_{N-1} \rangle$ spans more of $\mathcal{L}^2[0, 1]$ and tbe left-hand side of (13) must go to zero as $N \to \infty$, so long as it remains orthogonal to $\langle f_2, \cdots, f_{N-1} \rangle$.

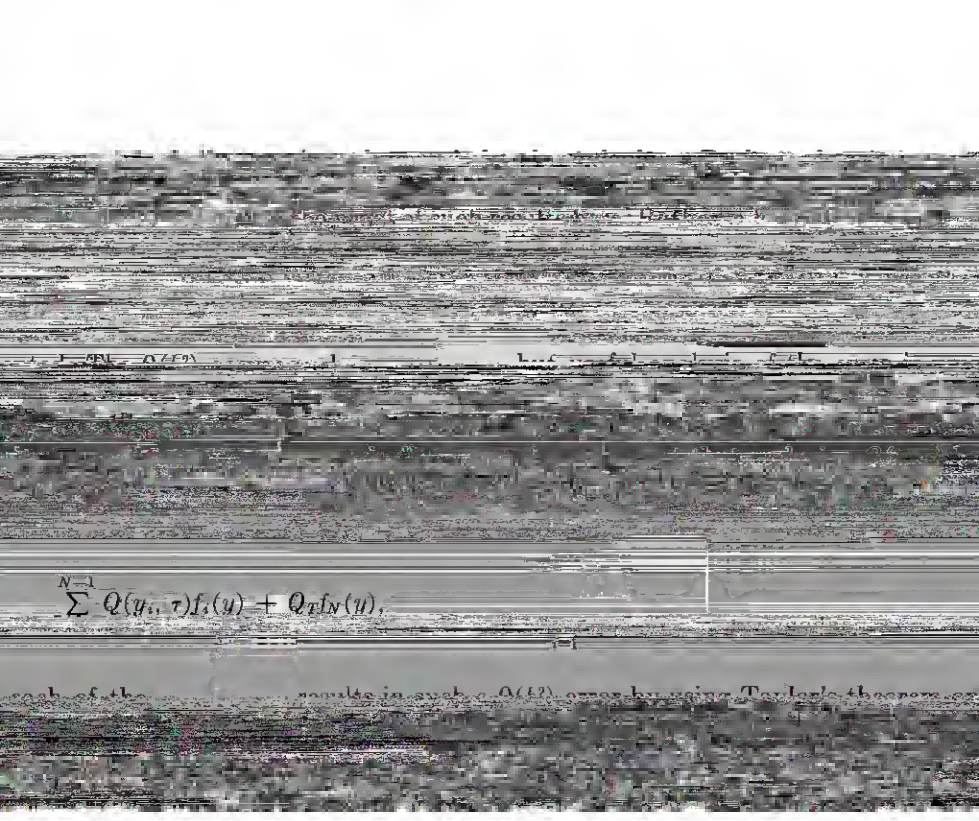
If we carry out the substitution of (15) and (16) into (14), with $f(y) = f_i(y)$, $2 \leqq i \leqq N - 1$, the $N - 2$ equations result:

$$\begin{aligned} \sum_{j=2}^{N-1} Q_j \left[\beta \int_0^1 f_j' f_i' dy - \sum_{k=1}^{N} \psi_k \int_0^1 f_j' f_k f_i dy + Q_T \int_0^1 f_j' f_i' f_N' dy \right] \\ + \tfrac{1}{2} \sum_{j,k=2}^{N-1} Q_j Q_k \int_0^1 f_j' f_k' f_i' dy + \sum_{j=2}^{N-1} \dot{Q}_j(\tau) \int_0^1 f_j f_i dy \\ = - \left[\frac{Q_T^2}{2} \int_0^1 f_i' (f_N')^2 dy + Q_T \left(\beta \int_0^1 f_i' f_N' dy \right. \right. \\ \left. \left. - \sum_{k=1}^{N} \psi_k \int_0^1 f_k f_N' f_i dy \right) \right]. \end{aligned} \tag{18}$$

we set $Q_i(m+1) = Q_i(m) + r_i(m)$, substitute this into (21), and linearize the resulting equations for the $r_i(m)$:

amount the solution produced if any is highly erratic and non-monotone, and may even be negative.

From (22a) to (22c) and (25), we see that



$$\sum_{i=1}^{N-1} Q(y_i, \tau) f_i(y) + Q_\tau f_N(y),$$

[redacted]

this problem was very small Δx choices by the extrapolation routines—

For such cases we have

$$\int_0^1 (f_j')^2 f_{j-1}' dy = -(h_j)^{-2}, \tag{57}$$

$$\int_0^1 (f_i)^2 f_i' dy = 0 \tag{58}$$

ions $f'_{\dots} df_i/dy_{\dots}$ In all these expressions

nial extrapolation to the limit of the result of the

By using polyno

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Order Accuracy for Nonlinear Boundary Value Problems," Numer. Math.
No. 5 (April 1972), pp. 394–430.